

Fig. 1

(AG AS AU BI BR C CA CD CL CO CU F FE GA H H+ HG I K LI MG MN MO N NA
 NI O P PB PT R S SB SE SI SN TC TE W X ZN BR-R C#C C#N C#O C-*
 C-AS C-BR C-C C-CL C-CO C-F C-FE C-H C-HG C-I C-MO C-N C-O C-P C-R C-S
 C-SE C-SI C-SN C-TC C-TE C-X C=C C=N C=O C=R C=S CL-CA CL-FE CL-HG
 CL-MG CL-PT CL-R H-CL H-N H-O HG-R I-I I-R K-I N#N N-* N-CO N-FE
 N-MG N-N N-NI N-O N-P N-PT N-R N-S N-SN N-X N-ZN N=N N=O N=P N=S O-*
 O-AS O-BI O-CA O-CL O-CO O-FE O-HG O-K O-MG O-NA O-O O-P O-R O-S O-SB
 O-SE O-SI O-SN O=AS O=CL O=O O=P O=S O=SE P-F P-S P=AU P=S P=SE S-AS
 S-AU S-F S-FE S-HG S-MO S-R S-S SE-SE)

Fig. 2

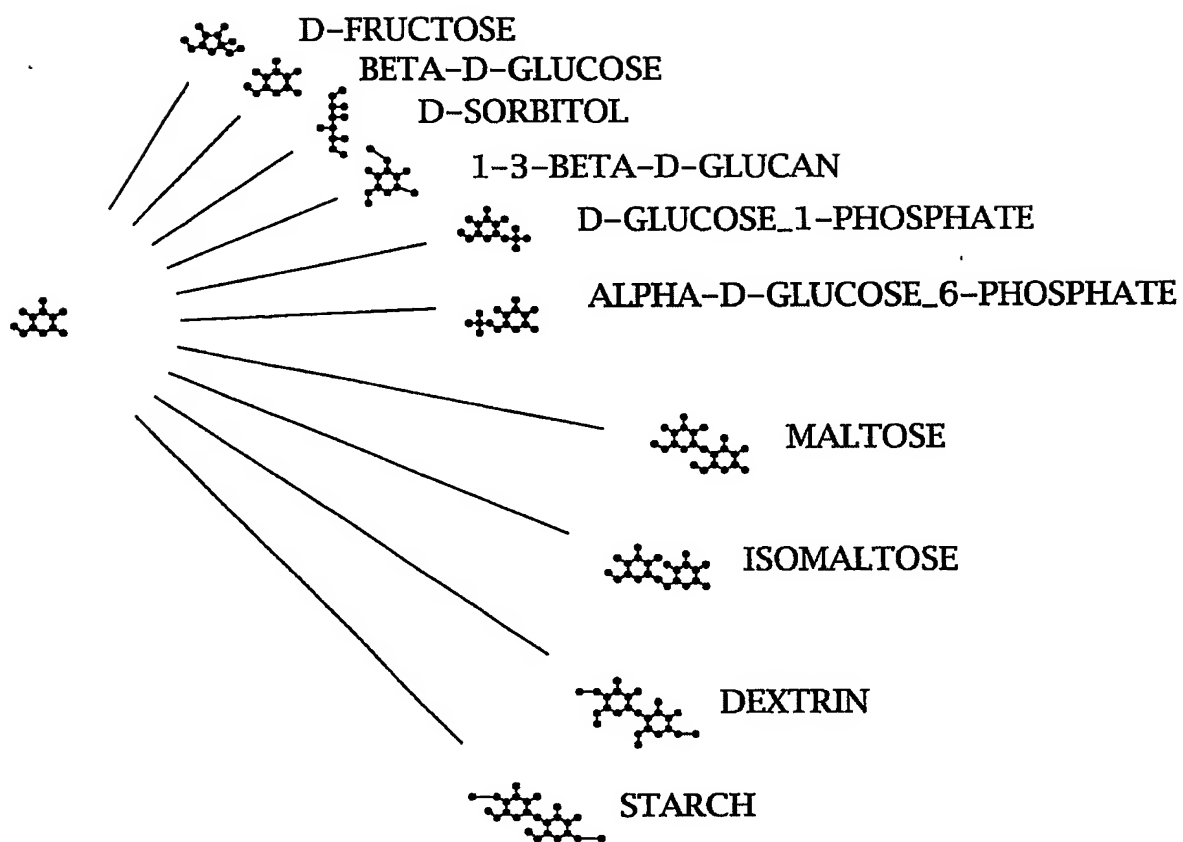


Fig. 3

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input    :  $\mathbf{x}^0, \mathbf{x}^L, F$ 
output   :  $\mathbf{P}^{0,L}$ 
begin
   $X \leftarrow (\mathbf{x}^0), \mathbf{P}^{0,L} \leftarrow ()$ 
  while  $X \neq ()$  do
     $\mathbf{x} \leftarrow \operatorname{argmax}(F(\mathbf{x}^i); \mathbf{x}^i \in X)$ 
     $\mathbf{T} \leftarrow \operatorname{successors}(\mathbf{x})$ 
    for  $\mathbf{x}^m \in \mathbf{T}$  do
      if  $\mathbf{x}^m = \mathbf{x}^L$  then
         $\mathbf{P}^{0,L} \leftarrow \operatorname{path}(\mathbf{x}^m)$ 
        return  $\mathbf{P}^{0,L}$ 
      if  $\mathbf{x}^m \notin X$  then
         $\operatorname{push}(\mathbf{x}^m, X)$ 
         $\operatorname{point}(\mathbf{x}^m, \mathbf{x})$ 
      else
        if  $F(\mathbf{x}^m) < F(\mathbf{x}^m)|_{old}$  then
           $\operatorname{point}(\mathbf{x}^m, \mathbf{x})$ 
    end
  end

```

Fig. 4

501a	Click here to indicate data file
502a	Click here to display and modify user-settable options
503	License and Intellectual Property Rights Statement Summary (Click here to view full statement)
504	Login Name: <input type="text"/> Password: <input type="password"/>
505a	Delivery Option 1 (Click Here To Select)
505b	Delivery Option N (Click Here To Select)

Fig. 5A

520	Your request has been accepted and is being processed
522	Your Results will be ready in approximately __ minutes
524	This request will be charged to account: AccountId (Click here to change account information)
526	The expected charge for this analysis is ____.
528	Results from this analysis will be transmitted to _____ (Click here to change results destination)

Fig. 5B

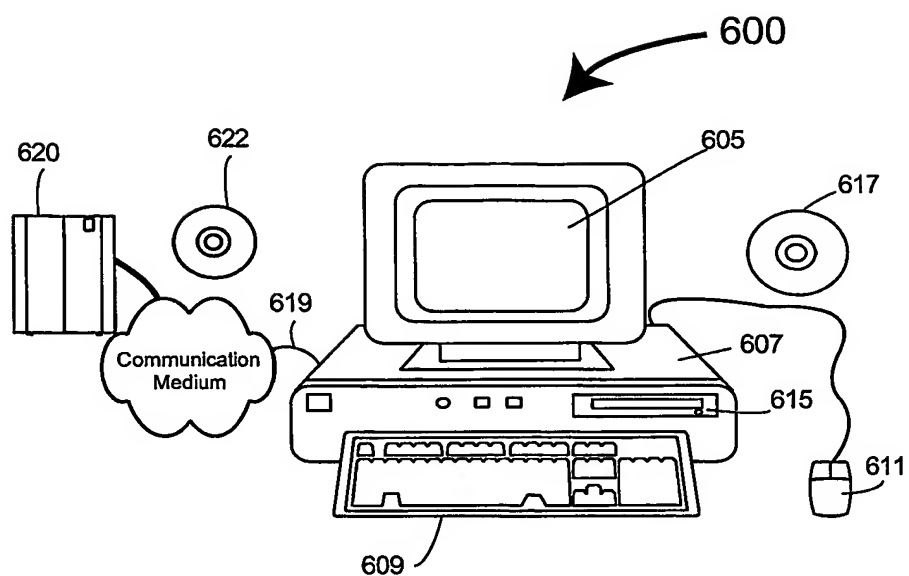


Fig. 6

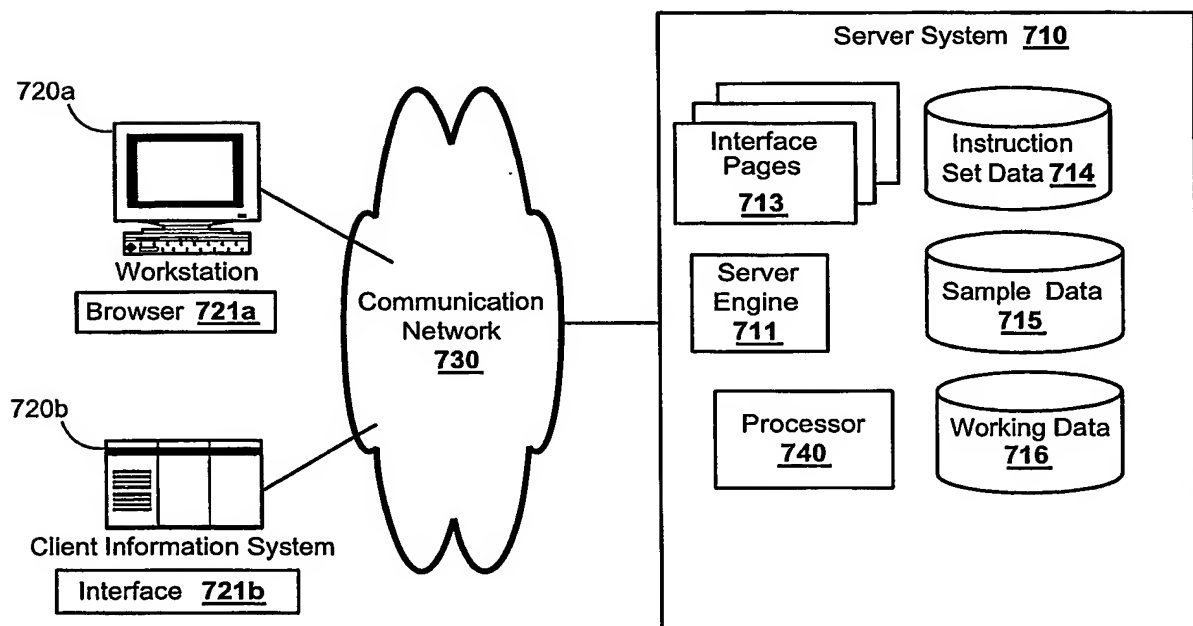


Fig. 7

Example (a)
From: α -D-Glucose
To : pyruvate

Alg	M	L	F	b*	t(s)
BFS	209	5	29	2.65	8.86
DFS	26	22	491	1.01	1.64
A*	27	6	29	1.44	1.83

Example (c)
From: α -D-glucose
To : 1,3-propanediol

Alg	M	L	F	b*	t(s)
BFS	652	7	81	2.33	19.42
DFS	19	17	185	1.01	1.83
A*	112	7	31	1.74	6.90

Example (b)
From: citrate
To : L-tyrosine

Alg	M	L	F	b*	t(s)
BFS	126	3	37	4.63	6.76
DFS	4718	123	2013	2.00	69.14
A*	20	6	13	1.34	1.98

Example (d)
From: citrate
To : L-histidine

Alg	M	L	F	b*	t(s)
BFS	653	6	45	2.73	16.97
DFS	-	-	-	-	$> 10^4$
A*	72	7	15	1.61	4.20

Fig. 8

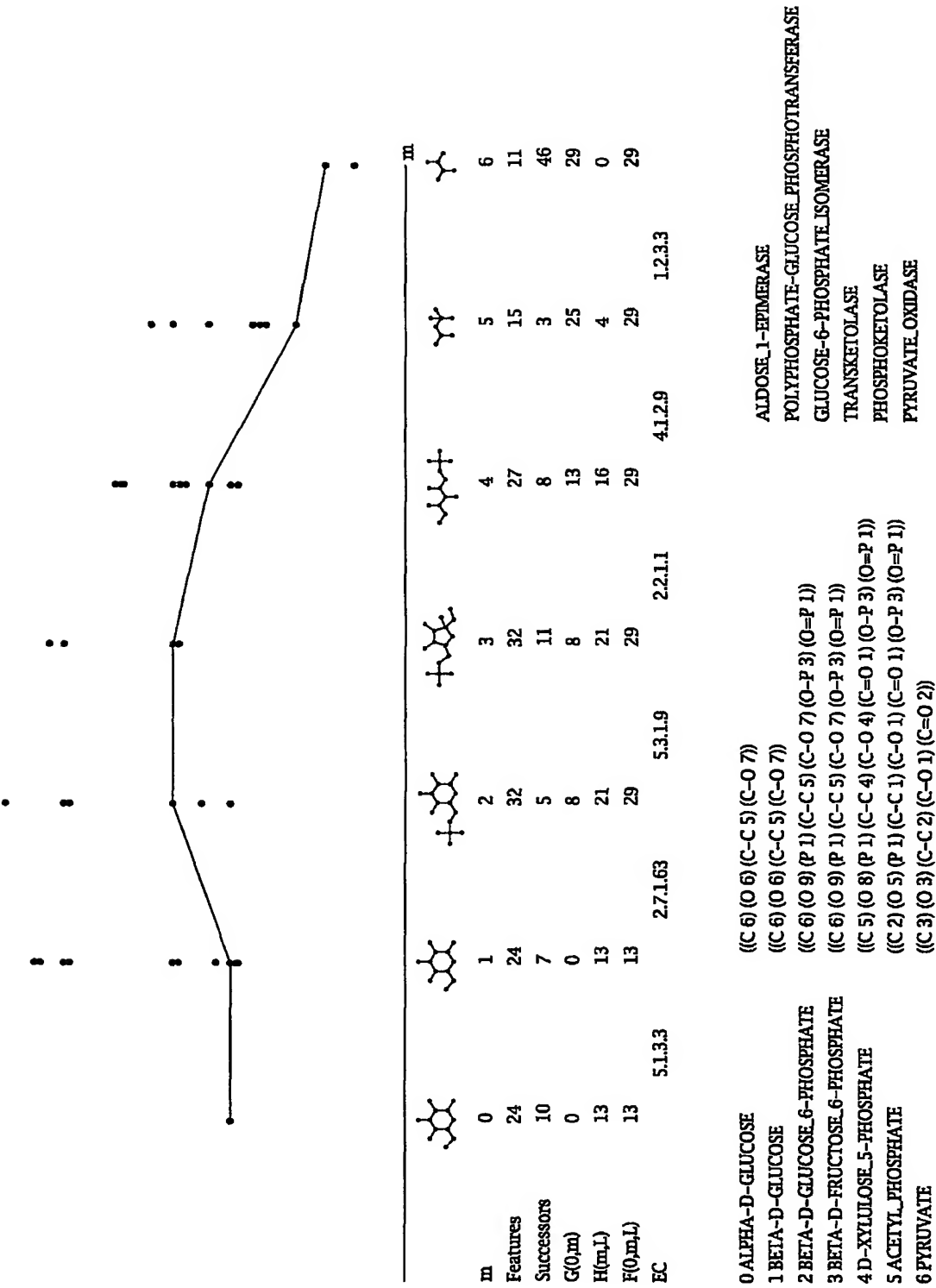


Fig. 9

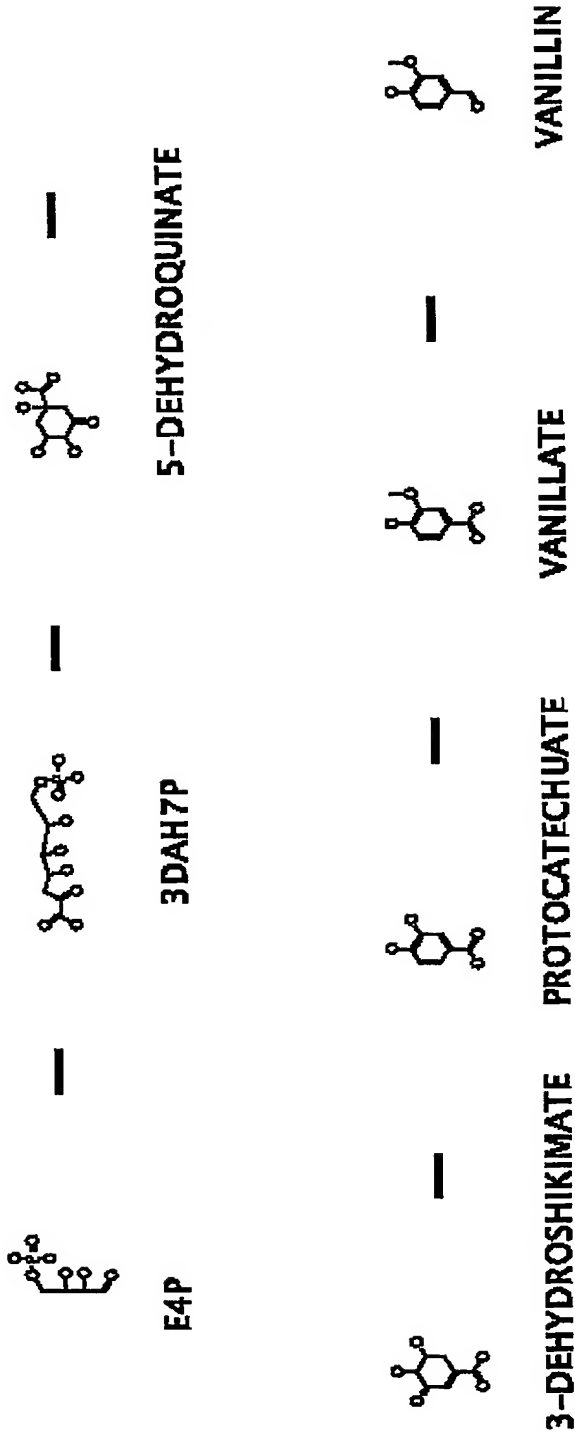


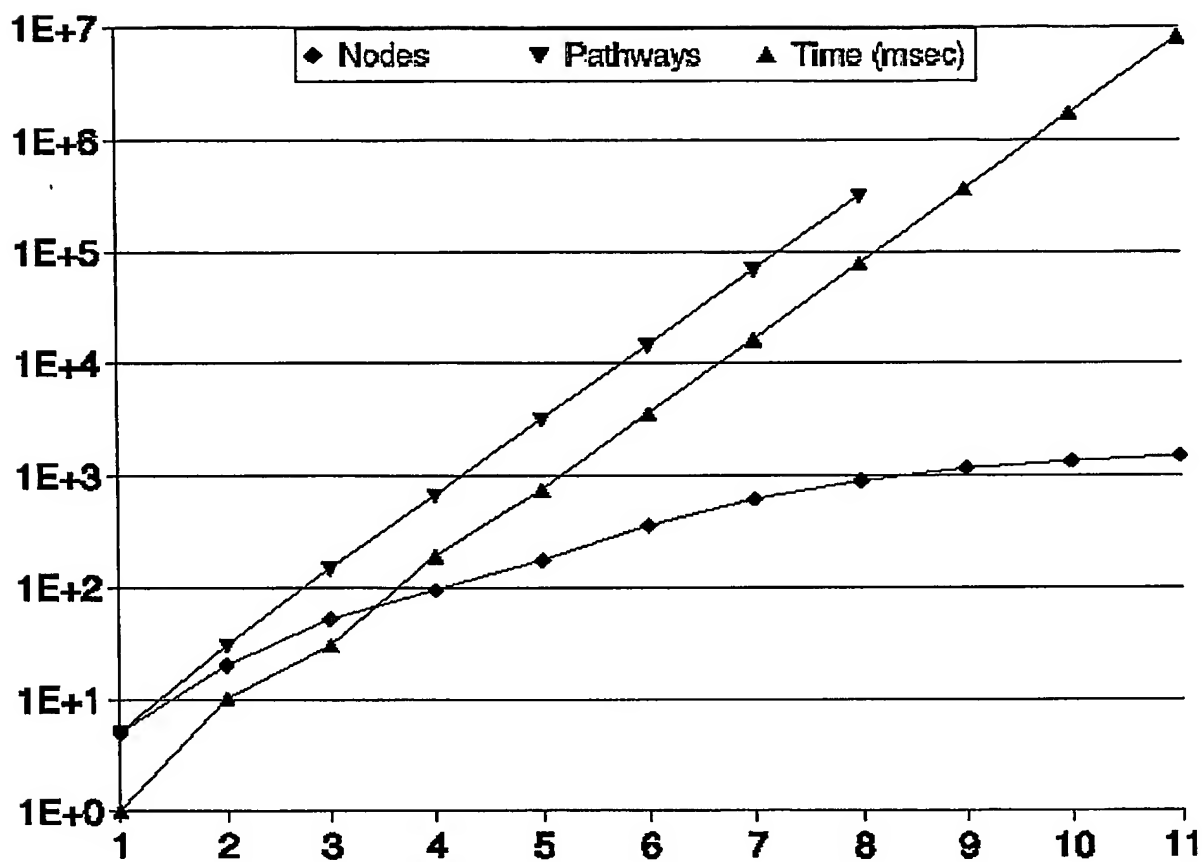
Fig. 10

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input :  $x^0, x^L, \Omega$ 
output:  $P^0, L$ 
begin
   $N \leftarrow \text{make-node}(x^0)$ 
  while  $N \neq ()$  do
     $n \leftarrow \text{pop}(N)$ 
     $P^0, L \leftarrow \text{node-solution}(n)$ 
    if goal-test( $n$ ) then
      return  $P^0, L$ 
    for ( $\text{reaction}, \text{compound}$ )  $\in \text{successors}(n)$  do
       $e \leftarrow \text{edge-cost}(n, \text{reaction}, \text{compound})$ 
       $h \leftarrow \text{h-cost}(\text{compound})$ 
       $g \leftarrow \text{g-cost}(n) + e$ 
       $f \leftarrow g + h$ 
       $d \leftarrow \text{depth}(n)$ 
       $n' \leftarrow \text{make-node}(n, \text{reaction}, \text{compound}, g, h, f, d)$ 
      push( $n', N$ )
     $N \leftarrow \text{sort}(N, f\text{-cost})$ 
end

```

Fig. 11



Variable	Regression
Nodes	$= 7.87 \times 1.73^x$
Paths	$= 1.23 \times 4.77^x$
Time	$= 0.31 \times 4.74^x$

Fig. 12

ALPHA-D-GLUCOSE + 2 ATP + 2R-2-HYDROXY-3-
PHOSPHONOXY-PROPANAL + PHOSPHENOLPYRUVATE +
NADH + OXYGEN + PYRUVATE + S-ADENOSYL-L-METHIONINE +
COA => ADP +D-XYLULOSE_5-PHOSPHATE + 2 ORTHOPHOSPHATE
+ 3 H2O + CO2 + NAD+ + S-ADENOSYL-L-HOMOCYSTEINE +
PRODUCTS_OF_ATP_BREAKDOWN + 4-HYDROXY-3-METHOXY-
BENZALDEHYDE +ACETYL-COA

Fig. 13

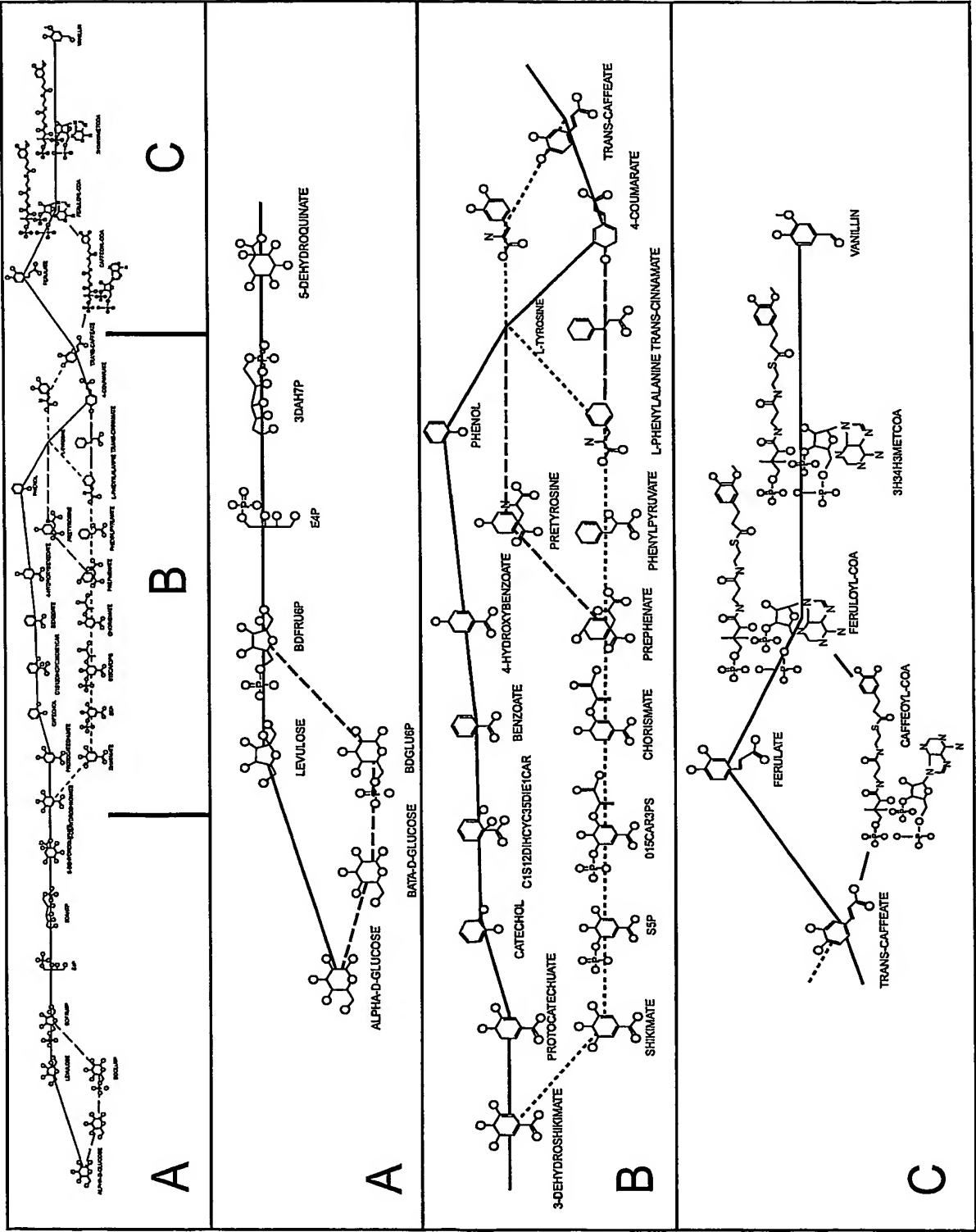


Fig. 14

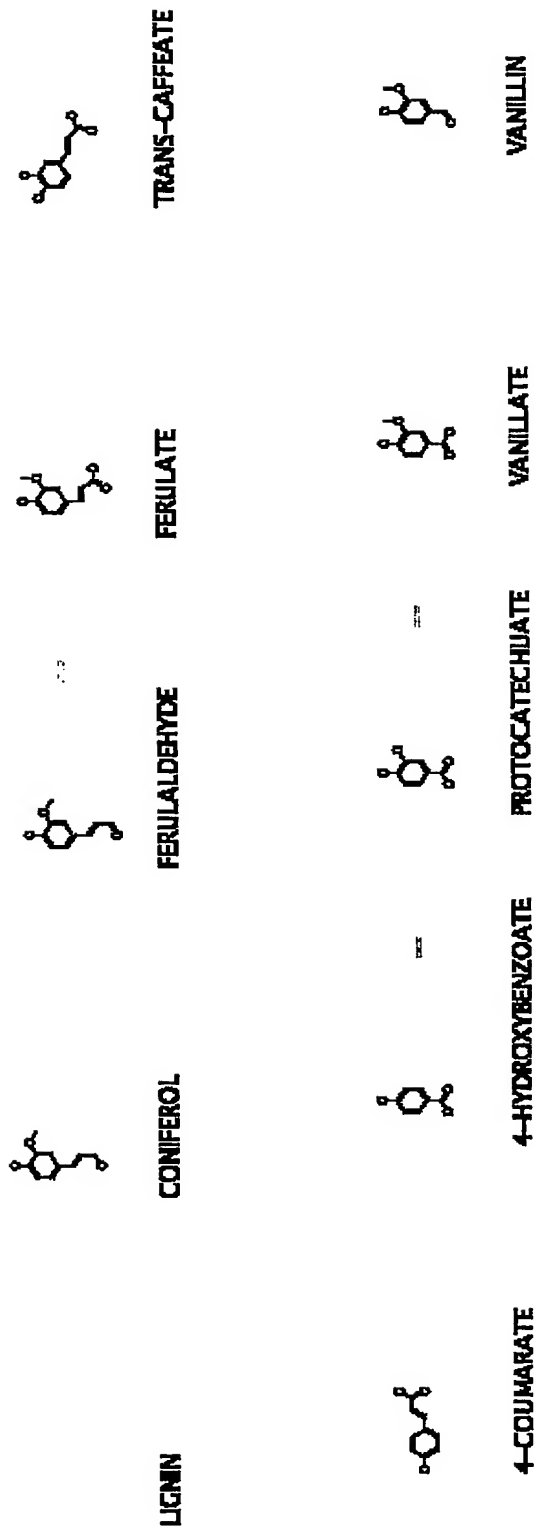


Fig. 15

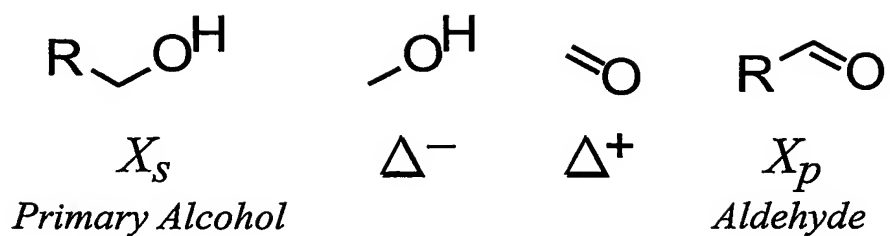


Fig. 16

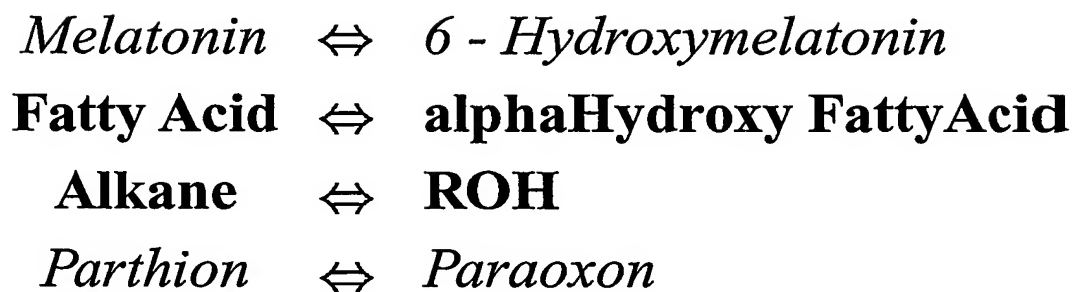


Fig. 17

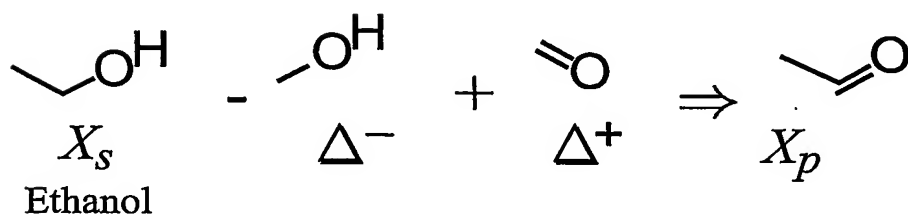


Fig. 18

```

input  :  $X_s$ , compound to metabolize
         $\bar{U}$ , list of rules
         $n$ , iterations

output : Graphical visualization

        Products
        Products  $\leftarrow \phi$ 
         $\Gamma_s \leftarrow \text{molecular-graph}(X_s)$ 
        for  $(\Delta^-, \Delta^+) \leftarrow \bar{U}$  do
        ┌  $\Gamma_p \leftarrow \text{graph-replace}(\Gamma_s, \Delta^-, \Delta^+)$ 
        │ if  $\Gamma_p$  then
        │  $X_p \leftarrow \text{find-compound-by-graph}(\Gamma_p)$ 
        │ if  $X_p = \phi$  then  $X_p \leftarrow \text{make-novel-compound}(\Gamma_p)$ 
        │ pushnew( $X_p, \text{Products}$ )
        └
        if  $n > l$  then
        ┌ for  $X$  in Products do
        │ └ append(metabolize( $X, \bar{U}, n-1$ ), Products)
        └

```

Fig. 19

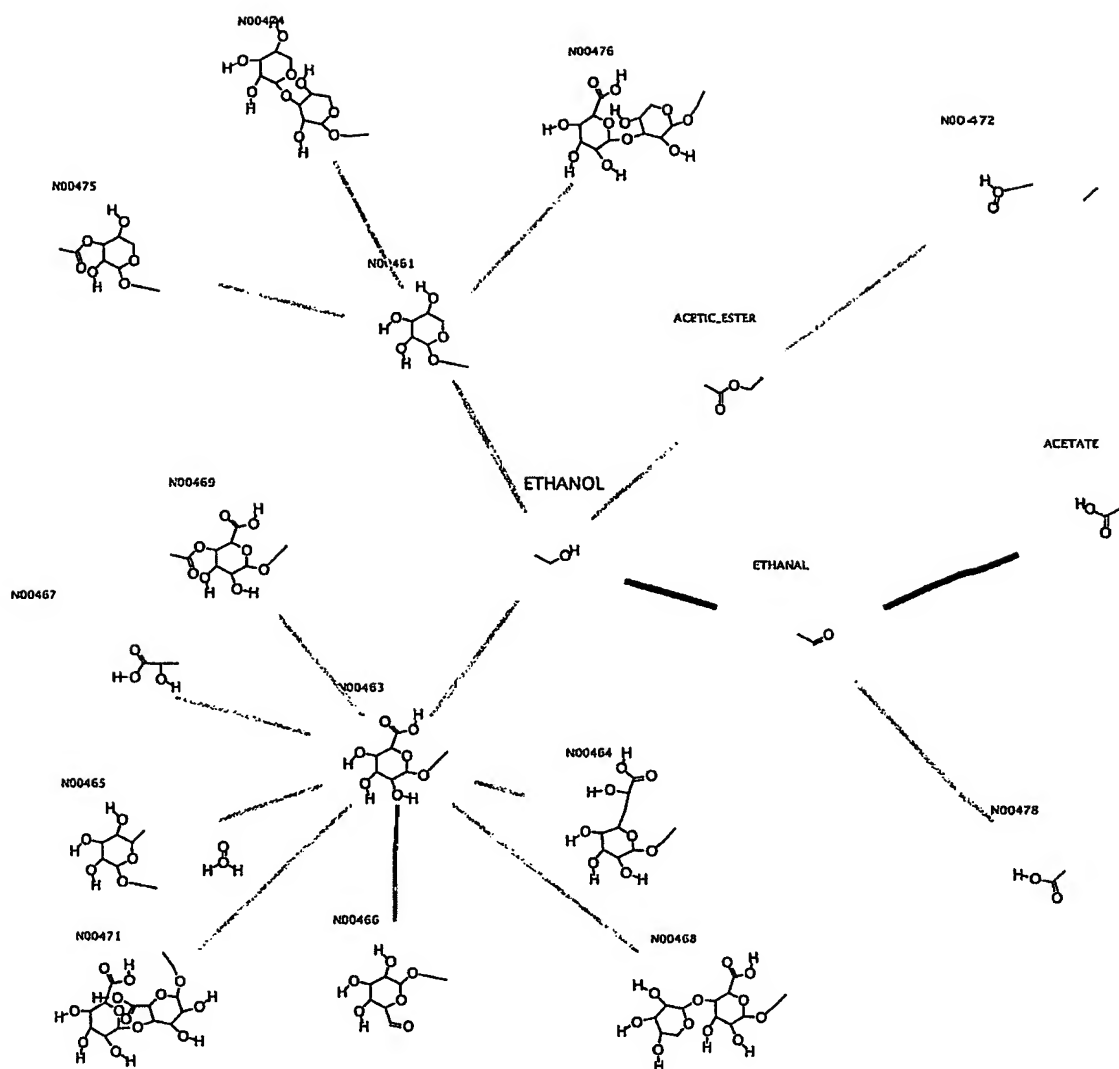


Fig. 20

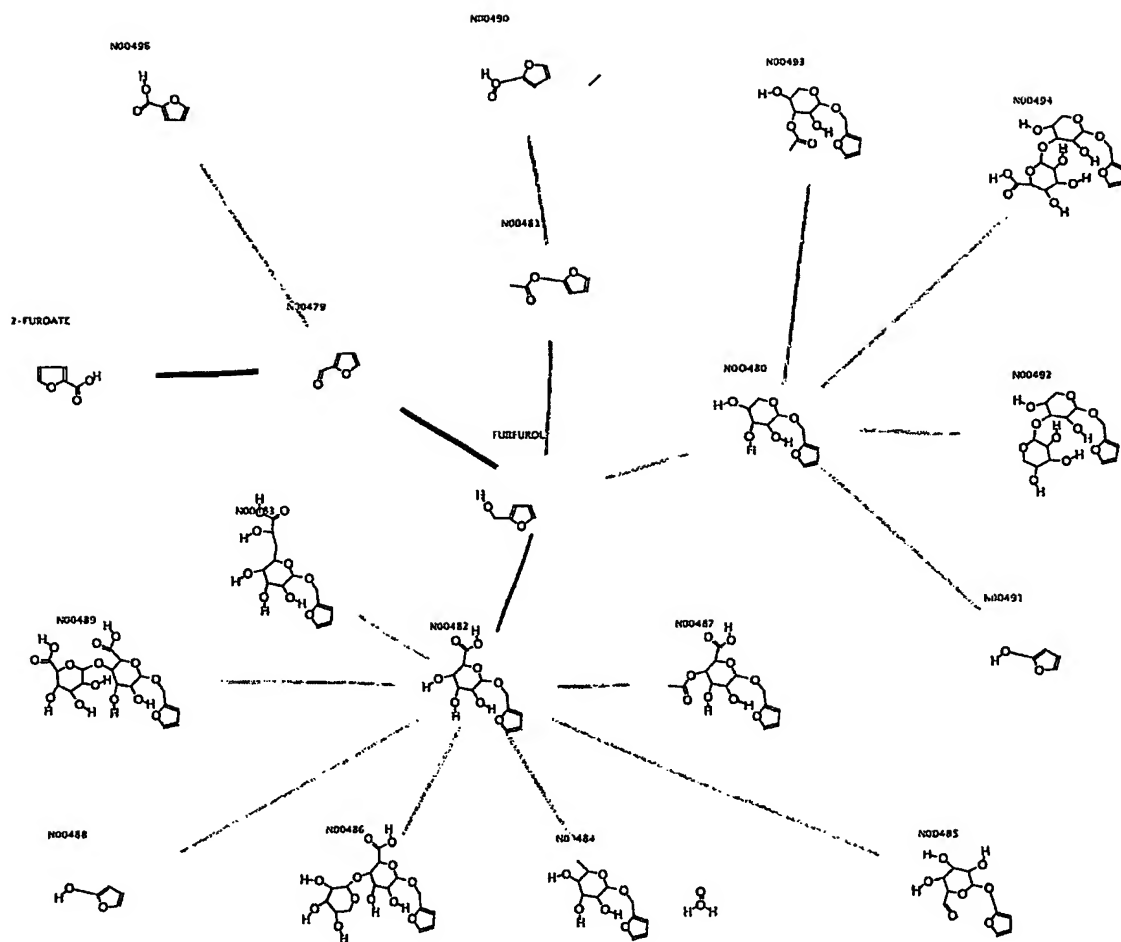


Fig. 21